Predicting Size-Resolved Particle Behavior in Multizone Buildings

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Abstract

We compare model predictions to measurements of SF_6 and environmental tobacco smoke particle concentrations in a three-room chamber experiment. To make predictions of multi-room aerosol transport and fate, we linked a multizone airflow model (COMIS) with an indoor aerosol dynamics model (MIAQ4). The linked models provide improved simulation capabilities for predicting aerosol concentrations and exposures in buildings. In this application, we found that the multizone air flow model was vital for predicting the inter-room airflows due to temperature differences between the rooms and when air-sampling pumps were operating during the experiment. Model predictions agree well with measurements, as shown by several comparison metrics. However, predictions of airborne ETS concentrations are slightly lower than measurements. This is mostly attributable to under-stating the source release amount, which we specified independently from literature estimates. Model predictions of ETS particle-size distributions agree with measurements; size bins with the peak concentrations are slightly over-predicted initially, but agree thereafter.

1.0 Introduction

Understanding the dynamic behavior of indoor aerosols is essential for accurately predicting their concentrations and fates within a building, and for estimating the human exposures. Processes such as coagulation, deposition, and removal by indoor filtration can depend strongly on the particle size distribution of the species, and these processes can affect the overall airborne concentration in buildings. The particle size distribution is also an important element in estimating the quantity and location of particle deposition in the lung.

Mathematical equations to express these processes in buildings, and computer software to solve them, have been developed and applied successfully for predicting aerosol concentrations in various indoor systems (for example Nazaroff and Cass (1989), Nazaroff et al. (1993), Miller and Nazaroff (2001)). Few studies, however, have applied these models to predict particle transport in multi-room buildings. A significant difficulty here is that the aerosol models require, as input, the airflows between the rooms and across the building shell for all HVAC operating conditions, wind conditions, and temperature differences between the rooms. Estimating these airflows experimentally can be costly or not possible in many cases; thus use of an indoor airflow model can be essential.

In recent years, researchers in the building sciences community have developed computer models that predict airflows in buildings. COMIS (Feustel, 1999) and CONTAM (Dols and Walton, 2002) are the two most widely used models, and are very similar in their mathematical foundations. Haghighat and Megri (1996) compared the models to each other, to data from laboratory experiments, and to data from field

experiments in a house. They report good agreement in each comparison. Sextro et al. (1999) applied the COMIS software to develop an airflow and tracer gas transport model for a three-floor building with an operating ventilation system. Model predictions agreed well with data under various ventilation scenarios.

With models to predict airflow improving in their robustness and general applicability, linking software to predict multizone airflows with software to predict size-resolved aerosol dynamics is an important advancement in the state of the art. To our knowledge, a linked set of models has not been described in the literature, nor exercised against data from experiments.

In this paper, we report on the linking of the COMIS multizone airflow model with the MIAQ4 aerosol dynamics model (Nazaroff and Cass, 1989). To demonstrate the application of the coupled models, we predict the transport of an inert tracer gas and environmental tobacco smoke (ETS) particles in a three-room chamber and compare predictions to field data. We show that the COMIS model was needed to predict the airflows through a partially open door and between rooms induced by zone-to-zone temperature differences and by operating air-sampling pumps; these flows were then input to MIAQ4.

2.0 Coupled airflow and aerosol transport

We use the COMIS airflow model (Feustel, 1999) to predict the airflows between rooms, and between indoors and outdoors. COMIS predicts the steady-state flow of air induced by wind, thermal buoyancy, and mechanical ventilation by representing a building as a collection of zones, connected by flow paths such as cracks, doors and

windows, and ductwork. Air is assumed incompressible, and airflow through these pathways is calculated by balancing pressure differences between the zones. Feustel (1999) and Lorenzetti (2002) describe the mathematical foundations of the model. The software has been applied to predict airflow and gas transport in multi-story, low- and high-rise residences (Feustel et al., 1985; Sextro et al., 1999), small office buildings (Feustel, 1990), controlled experimental test houses (Haghighat and Megri, 1996), and single-family houses (Haghighat and Megri, 1996, Zhao et al., 1998).

The outputs from COMIS are airflows between rooms and across the building envelope for every user-defined building operating mode and meteorological condition.

We then use the MIAQ4 aerosol dynamics software (Nazaroff and Cass, 1989) to predict the size-resolved transport and evolution of particle concentrations prompted by the COMIS-calculated airflows, and directed by particle dynamics behavior such as gravitational settling, coagulation, and thermal diffusion. MIAQ4 simulates a size- and chemically-resolved particle size distribution. It does not take into account evaporation, condensation, or homogeneous nucleation. The aerosol model was originally developed for and applied to predicting the behavior of particles from cigarette smoke in a chamber (Nazaroff and Cass, 1989) and of particulate matter in museums (Nazaroff et al., 1990).

The models are linked in a feed-forward manner. The airflows predicted by COMIS serve as inputs to MIAQ4. Feedback from MIAQ4 to COMIS is unnecessary since the total airflow mass is much greater than the pollutant mass, and can thus be ignored in the airflow mass balance equations.

We linked the models by writing a computer program that transforms output from COMIS into MIAQ4. We wrote the linking software in the Perl scripting language because the language contains several built-in functions for formatting text and numbers, and is available for most computer systems.

Since linking is in a feed-forward manner, the Perl script first runs COMIS for an entire simulation for all HVAC operations and meteorological conditions of interest. It then runs MIAQ4 in intermediate steps, halting the simulation to readjust the flow when changes in airflow or temperature conditions occur, and restarting it with the new state of the pollutant mass transport or loss.

3.0 Application: predict ETS particle transport in a three-room chamber

To demonstrate the linked software, we applied it to predict ETS particle transport in a three-room experimental chamber, and compared predictions to data. Apte et al. (2004) conducted tracer and ETS experiments in a full-scale, three-room, laboratory chamber. Figure 1 shows the floor plan of the chamber. For the experiments, side-stream smoke was produced by machine-smoked cigarettes in Room 2 for approximately eight minutes, while mainstream smoke was vented outside. Sulfur hexafluoride (SF_6) was injected simultaneously into Room 2 as a tracer gas. Small mixing fans were running in each room at all times to increase well-mixed conditions. A number of different experimental conditions were examined, and are reported in Apte, et al. For our purposes here, we chose an experiment where the door between Rooms 1 and 3 was open fully and the door between Rooms 2 and 3 was partially open (0.0254 meters). Both doors were standard height (2.12 meter). The temperature difference between

rooms varied from 0 to 1° C during the experiment. Air sampling tubes were installed in each room to draw air from the chamber to external analytical equipment. Gas- and particle-phase ETS tracer concentrations, ETS particle mass, and particle size distributions in each room were measured as a function of time. We refer the reader to Apte et al. (2004) for details of the experiments and analytical equipment; however a brief description of the tracer gas and particle measurement system is included here to provide context for discussion of the model-measurement comparisons.

3.1 Tracer gas and ETS particle characterization.

Data consisted of time-series and point measurements of 1) gas tracer concentrations, 2) total ETS mass concentration 3) size-resolved particle concentrations and 4) room air temperatures. Sulfur hexafluoride (SF_6) tracer gas was measured using a gas chromatograph with an electron capture detector (instrumentation details, including manufacturer and model numbers are given in Apte et al, 2004). Air was continuously drawn from each room (~1.8 m from the floor) at 1 L min^{-1}. The air samples were sequentially sent to the GC, resulting in measurements in each room every four minutes.

Total ETS particle mass was measured gravimetrically by particle collection on open face filters in each room connected to sampling pumps located outside the chamber. These samplers were taken for 30 min at 3, 6 and 24 h during the experiment. As discussed below, the intermittent operation of these particle-sampling pumps led to enhanced ventilation air flows in the chamber for which explicit account was needed to be taken into account in the modeling.

In addition, size- and time-resolved particle concentration measurements were provided by a Differential Mobility Particle Sizer (DMPS), which gave particle size measurements from 0.01 μm to 0.45 μm in diameter, and by an optical particle counter (OPC), which measured particle diameters from 0.09 μm to >3.5 μm. Total particle mass was also measured as a function of time by adding the masses collected on a 10-stage quartz crystal cascade impactor (QCM). These instruments all sampled from a continuously flowing sampling manifold connected to the center of each room. The DMPS and QCM provided data from each room every hour and the OPC provided data every three minutes.

3.2 Model-measurement comparisons

We developed a COMIS model of the three-room chamber with room dimensions, the size of door openings, and room temperatures (as a function of time) as model inputs. Because the experiments were run with the doors between the rooms open, we did not incorporate any added room-to-room leakages (e.g. cracks) in the model. We did include the air leakage between the chamber and the outside in the model, which we determined to be approximately 0.01 air changes per hour from tracer gas decay rate measurements, when the SF6 and DMPS/OPC sampler pumps were operating, but not the pumps for the open face filter samples. We distributed this leakage uniformly across the outer walls of the rooms

Figure 1 shows the predicted airflows at one instant in time during the experiment when the filter pumps were not running. The airflows change moderately over time due to changing room temperatures and, as we describe later, due to the

intermittent operation of the pumps for the aerosol filter samples. The airflow between Rooms 2 and 3 is significantly lower then the flow between Rooms 1 and 3 because the door between Rooms 2 and 3 is only partially open. At this instance in time, the very low flows move from Room 3 to the outside because of the minor temperature differences between them.

We used the airflow calculations to predict the dispersion of a puff release of 0.01 grams of SF_6 in Room 2 and compared the COMIS predictions to measurements (Figure 2). The COMIS model was not calibrated to the data; the input parameters, including size of the door opening between Rooms 2 and 3, were measured independently.

Figure 2 shows model-to-data comparisons with and without including the intermittent operation of the pumps to collect the total mass ETS particle samples at 3, 6 and 24 h. We note that the model inputs for the gas concentration predictions are not 'calibrated' by the experimental data. The figure shows that the sampling pumps, though the amount of air removed is small (4.5 to 4.8 m^3/h for 30 minutes), increase the ventilation rate of the chamber, causing an appreciable reduction in the observed concentration of SF_6 in the air. Because the overall leakage in the chamber is low, the pumping is a significant driver for air leakage when the pumps are operating. The inclusion of the air sampling pumps reduced the root mean squared error (RMSE) when comparing the predictions to the experimental data by 76% in zone 1 and 60% in zone 2. We also tested the sensitivity of the model to the size of the door opening between Rooms 2 and 3 in other model runs, and found openings larger or smaller than the actual measured opening size produced inferior concentration predictions.

The model-to-data comparison for Room 3 is similar to the comparisons for Room 1 because the door between them is completely open, and temperature differences between the rooms, though small, are predicted to generate large inter-room airflow, and thus mixing, between them. These model predictions are therefore also consistent with the data.

We next predicted the dispersion of ETS particles from smoking one cigarette in Room 2. Inputs to the MIAQ4 model were the airflow conditions predicted by COMIS, with inclusion of the intermittent use of the filter pumps, the chamber dimensions, measured temperatures as a function of time, and an emission rate profile for side-stream ETS particles, which we specified independent of the data from this experiment (Nazaroff et al., 1993) (Figure 3). We also specified the turbulence intensity factor for the chamber, which describes the stream-wise velocity gradient at the vicinity of the chamber wall (Crump and Seinfeld, 1981). In this application, we adjusted the turbulence intensity factor to calibrate the model predictions to the overall airborne ETS concentration data. We selected an intensity factor of 1.2 s^{-1}, which is consistent with values reported by Furtaw et al. (1996) and Lai and Nazaroff (2000).

Figure 4 shows the measured and modeled concentration of total ETS particles in Rooms 1 and 2, as measured by the filter samples and by the DMPS. The slopes of the decay curves are fairly consistent with the measured data, suggesting that, in general, MIAQ4 is properly predicting the transport and losses due to deposition and surface diffusion.

However, Figure 4 shows predicted particle concentrations, in general, lower than were measured (R^2=0.93, RMSE=52 ug/m^3). Since the SF_6 dispersion predictions

agree well with measurements, it is unlikely that the MIAQ4 is incorrectly predicting airflows. It is more likely that the actual ETS released during the experiment was larger than we assumed for input into the model (Figure 3) since the total side-stream particle mass emitted from a cigarette can vary from one experiment to the next (e.g., see Figure 12 in Apte et al.). It is also possible that the turbulence intensity factor chosen for the model was not correct, thus under-predicting particle deposition onto surfaces, and therefore underestimating these losses. Further experiments and modeling will be needed to determine the cause of the differences, but such analysis was beyond the purposes of this demonstration.

Figures 5 and 6 shows MIAQ4-predicted concentrations of ETS in Room 2 resolved by particle size compared to DMPS measurements at 40, 160, 460, and 640 minutes after the cigarette was smoked. Figures 7 and 8 shows model-to-data comparisons for Room 1. In general, the overall shapes of the model predictions agree well with the data. The difference between modeled and measured binned particle concentrations is consistent with the discrepancies in total concentrations shown in Figure 4. The size-resolved plots also show that relative differences between the measured and modeled are small and that across particle size and concentration no consistent biases exist in the model's predictions.

4.0 Discussion and concluding remarks

We have linked the COMIS multizone airflow model with the MIAQ4 aerosol dynamics model to predict size-resolved aerosol transport in multi-room buildings. Though both models have been reported and demonstrated individually in the

literature, they have not been applied together to predict size-resolved aerosol transport in multi-room buildings, or compared to real data. The linked model will be a useful tool for examining the behavior of aerosols in multizone buildings and predicting concentrations and exposures as a function of particle size. The latter may be especially important for evaluating different strategies for reducing aerosol exposures within buildings. The models can also be used to aid in the design and interpretation of field experiments.

As proof of concept, we applied the models to predict the transport and behavior of tracer gas and ETS particles measured in a three-room chamber. We obtained excellent agreement between the predicted and observed tracer gas concentrations in all three rooms. The predictions of both ETS particle mass and size-resolved particle concentrations also agreed well with the measurements. COMIS was particularly helpful for estimating the inter-room airflows caused by operating the filter-sampling pumps, and therefore reduced the number of experiments needed to characterize the airflows.

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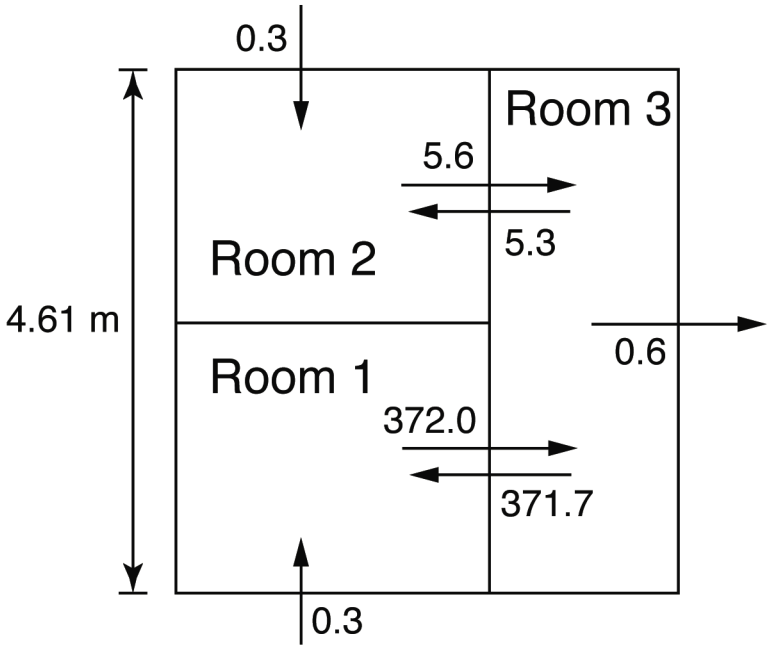

Figure 1: Floor plan of the experimental chamber. The arrows indicate the direction of the predicted airflows and their magnitude [m^3/hr]. These estimates are for a time when the intermittent aerosol-sampling pumps were not operating. The airflows change during the experiment according to temperature differences between rooms, and whether air-sampling pumps were operating to collect ETS particle measurements. The door between Rooms 1 and 3 is open fully and the door between Rooms 2 and 3 is open partially. The cigarette was machine smoked in Room 2 to generate ETS.

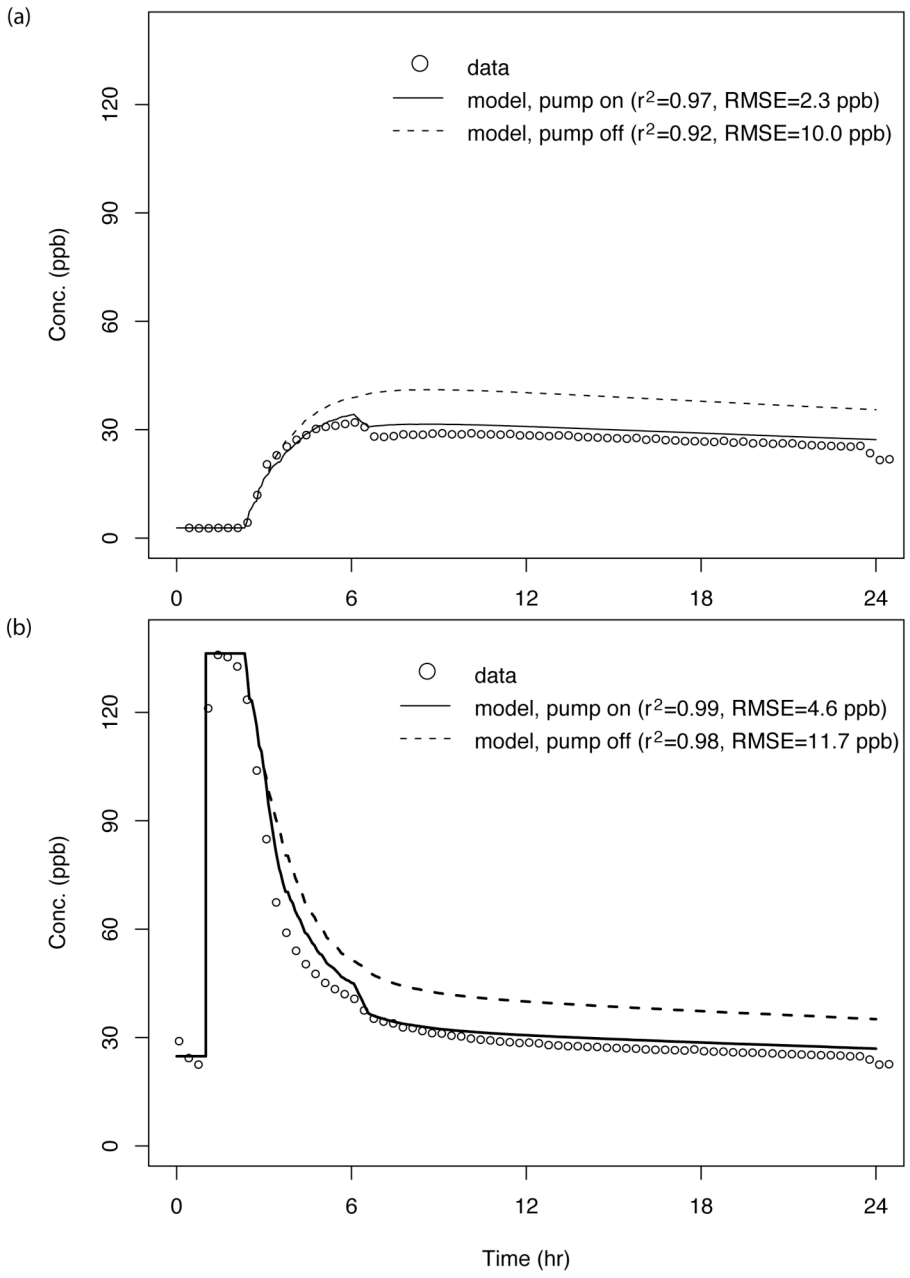

Figure 2: SF_6 concentration measurements compared to model predictions in (a) Room 1 and (b) Room 2 (source room). "Pump on" refers to COMIS predictions that included operation of the intermittent air sampling pumps at t=3, 6 and 24 hours to collect ETS particle measurements. The pumps ran for 30 min at each sampling time. The model predictions for Room 3 are similar to those for Room 1. We measured SF_6 every 4 minutes, though for clarity, we plotted data every 20 minutes.

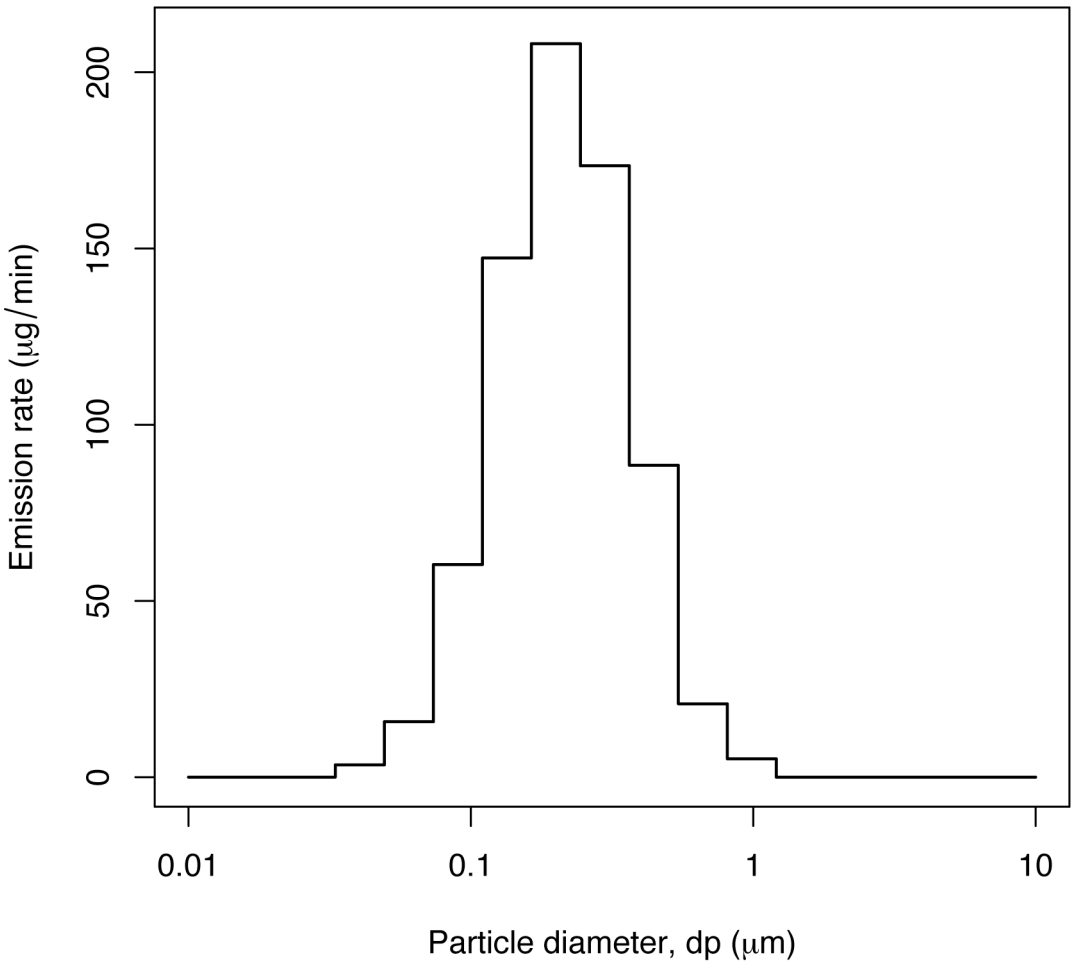

Figure 3: Size-resolved emission rate profile for side-stream ETS particles used as input to the MIAQ4 model (from Nazaroff et al., 1993). The overall emission rate is approximately 723 ug/min.

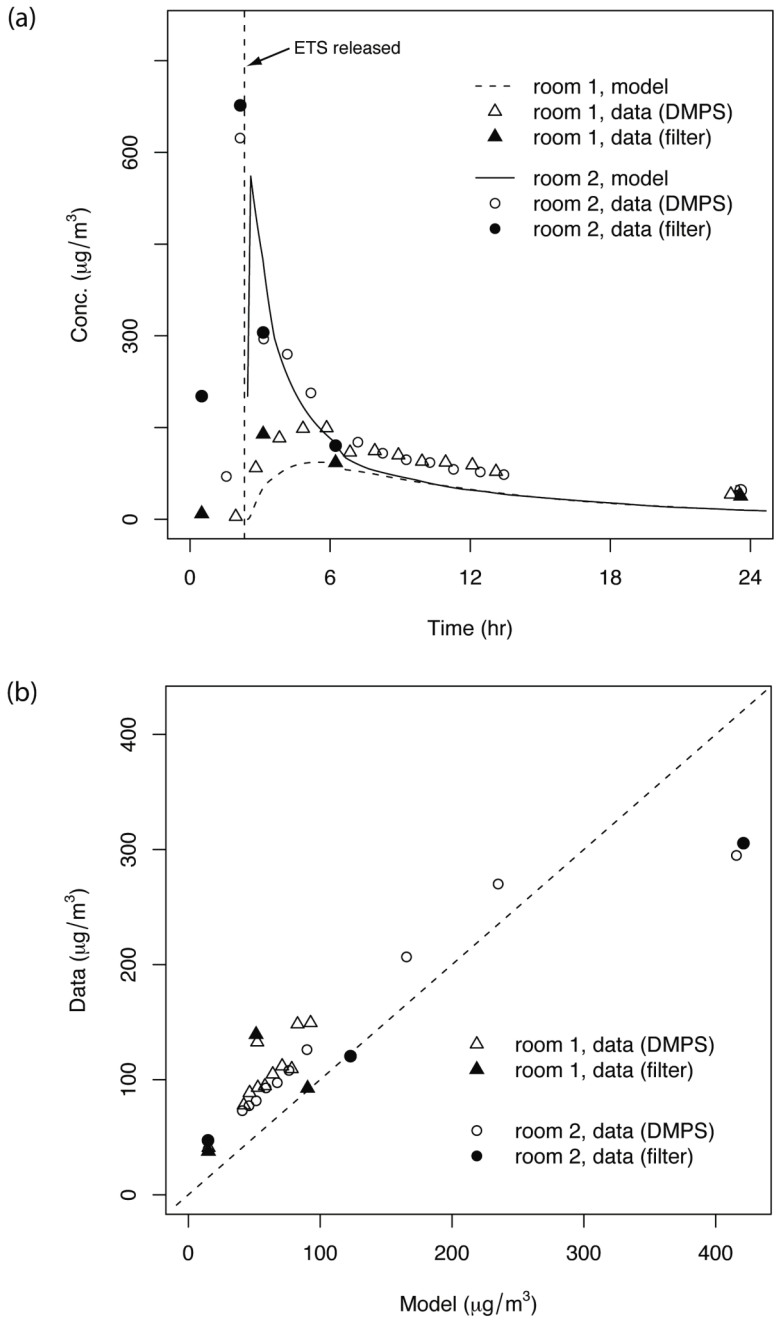

Figure 4: Time-series total ETS mass measurements and model predictions are shown in (a). Total measured ETS particle concentration compared to model predictions (R^2=0.93, RMSE=52 ug/m^3) are shown as a scatter plot in b). The model predictions for Room 3 are similar to the predictions for Room 1. The cigarette was emitted in Room 2. Measurements before the ETS release are background from earlier experiments.

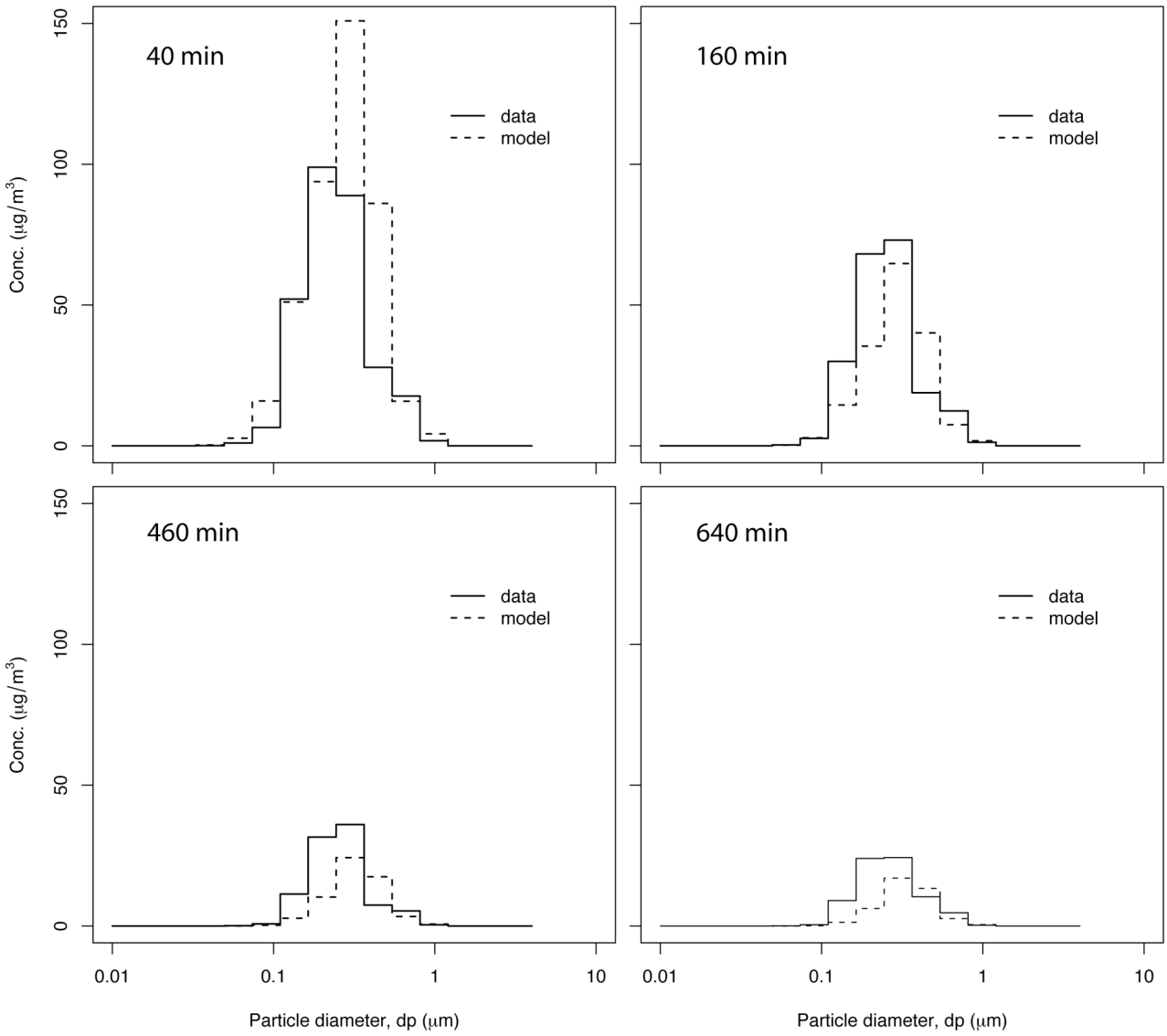

Figure 5: MIAQ4-predicted concentrations of ETS particles in Room 2 compared to DMPS measurements resolved by particle size, 40, 160, 460, and 640 minutes after emitting side-stream ETS.

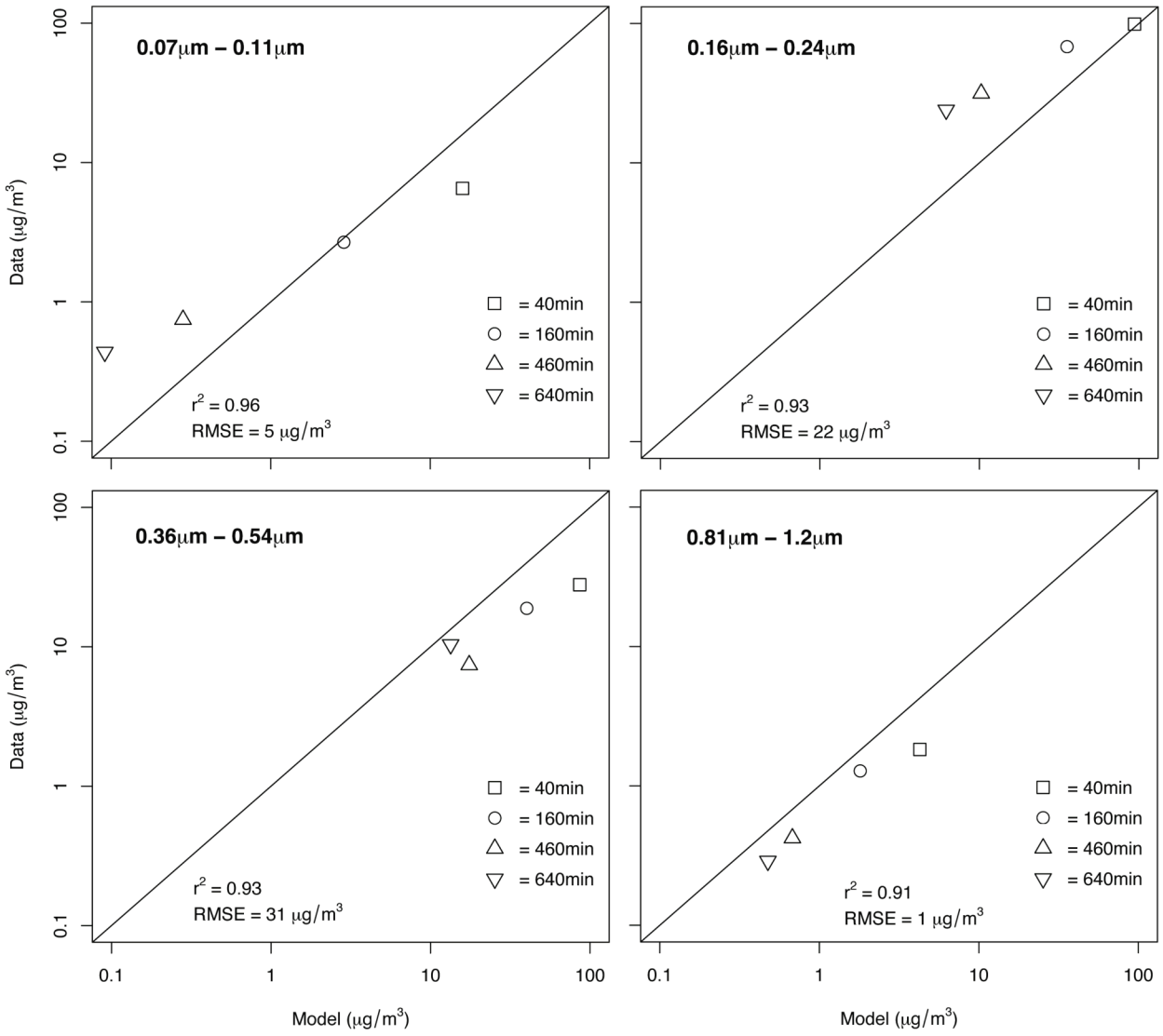

Figure 6: Comparison of model predictions to DMPS measurements in Room 2 for four particle sizes. The full profiles are shown in Figure 5 (note: the y-axis scale differs from Figure 5).

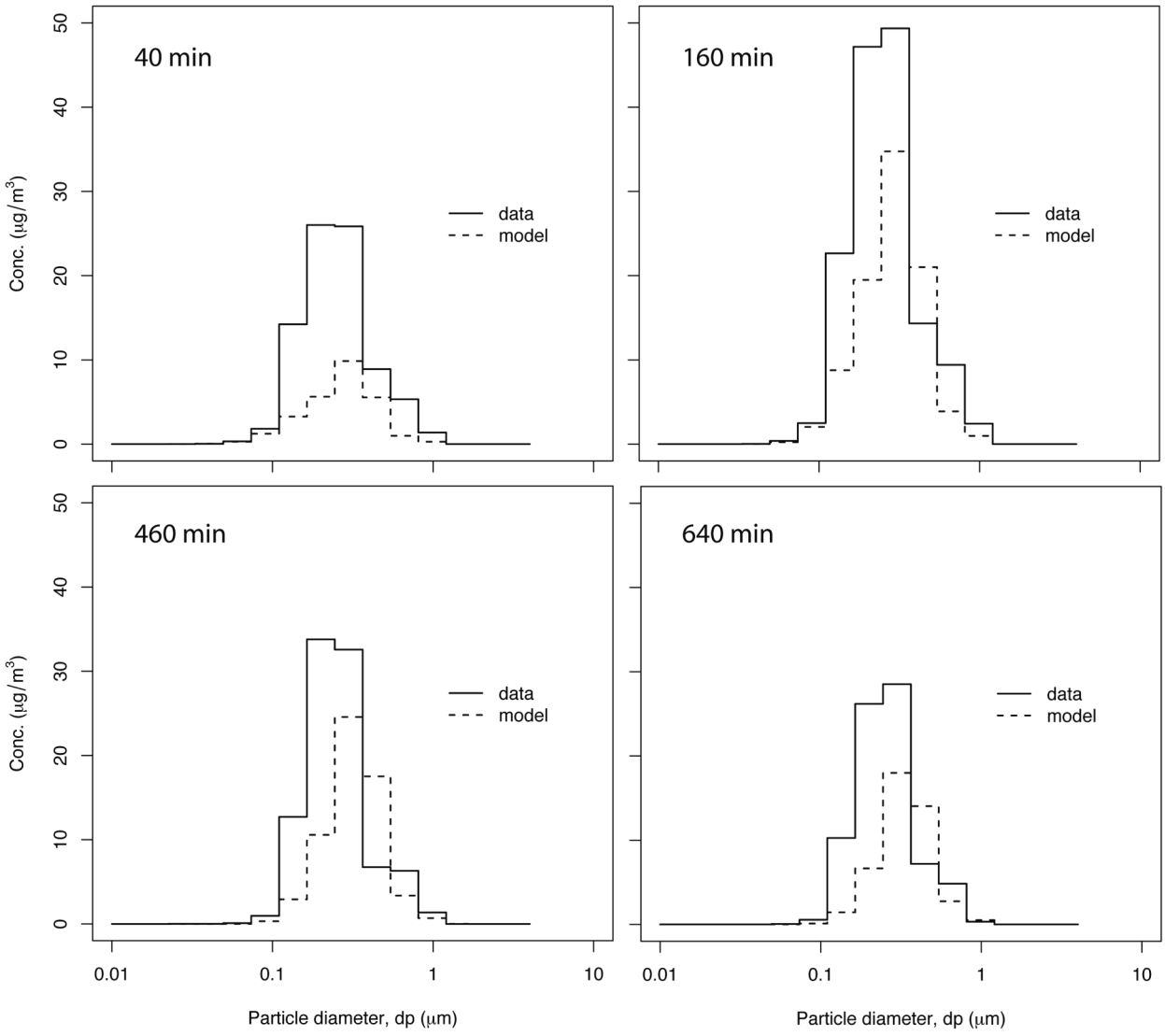

Figure 7: MIAQ4-predicted concentrations of ETS particles in Room 1 compared to DMPS measurements resolved by particle size, 40, 160, 460, and 640 minutes after emitting side-stream ETS.

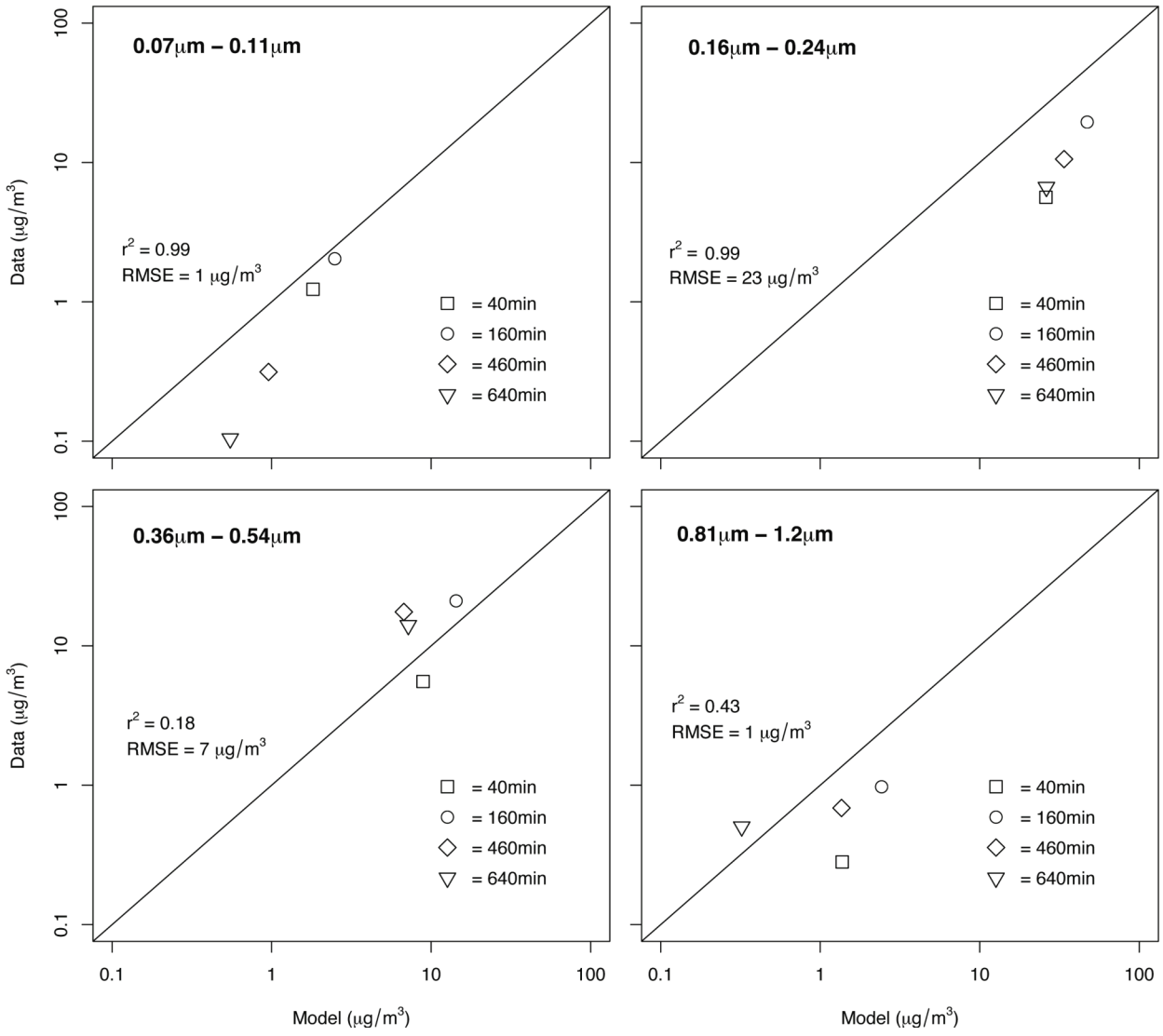

Figure 8: Comparison of model predictions to DMPS measurements in Room 1 for four particle sizes. The full profiles are shown in Figure 7. (note: the y-axis scale differs from Figure 7).